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Fast and Accurate CBR Defense for Homeland Security: Bringing HPC to the First Responder and Warfighter

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Abstract

An urban-oriented emergency assessment system for airborne Chemical, Biological, and Radiological (CBR) threats, called CT-Analyst[®] and based on new principles, gives greater accuracy and much greater speed than possible with current alternatives. The increased accuracy derives from detailed, three-dimensional (3D) computational fluid dynamics (CFD) computations including, solar heating, buoyancy, complete building geometry specification, trees, and wind fluctuations. A limited number of such detailed high performance computing (HPC) computations for a given area can be extended to all wind directions and speeds, and all likely sources and source locations using a new data structure called Dispersion Nomographs[™]. By performing all the heavy computing ahead of time using the full power of HPC parallel platforms well suited to the application, the results of a number of complete, high-resolution 3D simulations can be recalled for operational usage with no sensible delay for integration of even simple models. In this way, we have solved the usual dilemma of more computer time being required to obtain better answers. The best available answers can be presented instantly with full urban geometry in a readily comprehended format.

1. Introduction

The emergence of increasingly powerful computers stimulated the development of obstacle-resolving micro-scale flow and transport models based on CFD. In recent years, these types of models are playing an important role in many applications. They serve as general tools in fluid engineering and wind engineering when complex flow systems have to be designed. Under the general category of Urban Aerodynamics^[1], these models are now commonly applied to predict contaminant transport (CT) in complex structured urban landscapes. Use of such

models is made in the licensing of new industrial plants, in safety analysis studies for accidental releases of hazardous materials in the chemical industry, or in the context of crisis management after terrorist attacks or accidents in urban environments.

Urban airflow accompanied by CT presents new, extremely challenging modeling requirements^[2] best met using complex-geometry simulation tools developed by the aerospace industry. Configurations with complex geometries and unsteady buoyant flow physics are involved. The wide range of temporal and spatial scales rapidly overwhelms the current modeling capacities. Crucial technical issues that need to be addressed include time-dependent turbulent fluid transport (aerodynamics), environmental boundary condition modeling (meteorology), and the practical post-processing of the simulation results for use by responders in actual emergencies. The advantages of the CFD approach and the large eddy simulation (LES) representation include the ability to quantify complex geometry effects, to predict dynamic nonlinear processes faithfully, and to treat turbulent problems reliably in regimes where experiments, and therefore model validations, are impossible or impractical.

CFD solutions to CT can be highly accurate, but are too slow for emergency response purposes. One practical solution to this critical dilemma carries out the unsteady CFD simulations in advance and pre-computes compressed databases for specific urban areas incorporating suitably parameterized weather for a full set of wind conditions and distributed test-sources. The relevant information is summarized as *Dispersion Nomograf[™]* datasets^[3] so that it can be used in a portable system called Contaminant Transport Analyst (CT-Analyst[®])^[4] that reproduces the CFD quality-results nearly instantaneously with little loss of fidelity.

This paper presents this new methodology that brings the fidelity and accuracy of CFD to the first responder or warfighter at speed necessary for emergency response. It.

presents an overview of the issues involved in meeting these seemingly contradictory requirements

A. Standard CFD Simulations

Some “time-accurate” flow simulations that attempt to capture the urban geometry and fluid dynamic details are a direct application of standard (aerodynamic) CFD methodology to the urban scale problem. An example is the finite element CFD simulations of the dispersion of a contaminant in the Atlanta, Georgia metropolitan area^[5]. The model includes topology and terrain data and a typical mesh contains approximately 200 million nodes and 55 million tetrahedral elements. These are grand-challenge size calculations and are run on 1,024 processors of a Cray T3E taking up to a whole day to run. Similar approaches are being used by other research groups^[6,7]. The chief difficulties with this approach for large urban regions are that the solutions are very computer intensive (days or weeks) and involve severe overhead associated with mesh generation.

B. The LES Approach for Contaminant Transport

Direct numerical simulation (DNS) is prohibitively expensive for most practical flows at moderate-to-high Reynolds number, and especially so for urban CT studies. On the other end of the CFD spectrum are the classic aerodynamic methods such as the Reynolds-Averaged Navier-Stokes (RANS) approach, which simulate the mean flow and approximately model the effects of fluctuating scales^[8]. These approaches are typically unacceptable for urban CT modeling because they are unable to capture the inherently unsteady but coherent plume dynamics driven by the urban geometry. Large eddy simulation (LES) constitutes an effective intermediate approach between DNS and the RANS methods^[9]. LES is capable of simulating flow features that cannot be handled with RANS such as significant flow unsteadiness and localized vortex shedding, and provides higher accuracy than the industrial methods, but at a lower cost than DNS. LES solutions converge to the solutions of the Navier-Stokes equations as resolution is increased, whereas RANS generally do not. Because the larger-scale unsteady features of the flow govern the unsteady plume dynamics in urban geometries, therefore, the LES approximation can capture key features which the RANS methods and the various Gaussian plume methodologies cannot. Moreover, given its potential for higher computational efficiency, the Monotone Integrated LES (MILES) approach (see Reference 10 for a recent review) is well suited for CFD-based plume simulation

for urban-scale scenarios, an application where classical LES methods are expensive.

A practical example of urban-scale MILES is depicted in Figure 1 which shows contaminant dispersion in Times Square, New York City. The figure demonstrates the typical complex unsteady vertical mixing patterns caused by building vortex and recirculation patterns, and the predicted associated endangered region associated with this particular release scenario. The large variability of concentration values from minute to minute is evident and thus the need for unsteady, time-dependent simulation models.

C. The FAST3D-CT Model

The FAST3D-CT 3D urban aerodynamics model^[3,11,12] is based on the scalable, low dissipation Flux-Corrected Transport (FCT) convection algorithm^[13,14]. FCT is a high-order, monotone, positivity-preserving method for solving generalized continuity equations with source terms. The version of the convection algorithm implemented in FAST3D-CT is documented in References 15 and 16. Relevant physical processes simulated in FAST3D-CT include complex building vortex shedding, flows in recirculation zones, and approximating the dynamic subgrid-scale turbulent and stochastic backscatter. The model also incorporates a stratified urban boundary layer with realistic wind fluctuations, solar heating including shadows from buildings and trees, aerodynamic drag and heat losses due to the presence of trees, surface heat variations and turbulent heat transport.

Modeling a pollutant as well mixed globally is typically not appropriate in problems where short time spans and large air volumes are involved. It is important to capture the effects of unsteady, buoyant flow on the evolving pollutant concentration distributions. In typical urban scenarios, both particulate and gaseous contaminants behave similarly insofar as transport and dispersion are concerned, so that the contaminant spread can usually be simulated effectively based on appropriate pollutant tracers with suitable sources and sinks. In other cases, the full details of multigroup particle distributions are required. Additional physics include multi-group droplet and particle distributions with turbulent transport to surfaces as well as gravitational settling, solar chemical degradation, evaporation of airborne droplets, re lofting of particles on the ground and ground evaporation of liquids. Details of the physical models in FAST3D-CT are given in Reference 16 and omitted here for brevity. The primary difficulty is the effective calibration and validation of all these physical models since much of the input needed from field measurements of these processes is typically insufficient or even nonexistent.

2. Fast and Accurate CBR Defense

A typical run with the FAST3D-CT model for a complex urban area of 30 square km resolved with 6 m cells takes 24 hours on a 16-processor SGI computer system. This is significantly faster per square km than classical CFD models due to the savings achieved by MILES and other algorithmic improvements. The *critical* dilemma in the CT application is that unsteady urban-scenario flow simulations are currently feasible—but they are still expensive and require a degree of expertise to perform. Troops in the field, first responders, and emergency managers on site to cope with contaminant release threats have perhaps a minute to make decisions and cannot afford to wait while actual simulations and data post-processing are carried out either locally or remotely.

An operational solution of this dilemma carries out unsteady CFD simulations in advance and pre-computes compressed databases for specific urban areas incorporating relevant meteorology and a full set of wind conditions and distributed test-sources. The relevant information is summarized as *Dispersion Nomograf*[™] datasets^[3] so that it can be directly applied locally on portable computers with sensors and verbal reports providing current information regarding local presence of contaminants, contaminant concentrations, and winds. Thus there is now a methodology making 3D CFD really useful for crisis managers in real time, operational situations. The accuracy of CFD simulations is recovered nearly instantly with little loss of fidelity. The current implementation of this new approach is called CT-Analyst^{®[4]}. Near instantaneous CT assessment with high-fidelity can reduce the number of people being exposed in urban areas, even for large crowds out in the open, by up to a factor of six once a simple sensor or reporting network is in place. First responders and headquarters staff can use CT-Analyst displays for data fusion to give a minute-by-minute situation assessment.

A. Nomograf Description

Nomographs[™] are new, compact, pre-computed data structures that capture the aerodynamic and turbulent effects of terrain, buildings, vegetation and surface types on contaminant plume transport and dispersion. Using nomographs, improved accuracy and much greater speed are achieved for urban-oriented emergency assessment. By interpolating into these patented data structures, we can perform plume predictions in complex geometry and related assessments in milliseconds for wide areas with complex terrain such as cities, military bases, and important facilities.

The Naval Research Laboratory's (NRL's) FAST3D-CT CFD model, as described above, underpins our current implementation of dispersion nomographs. FAST3D-CT computes the multi-gigabyte 3D, contaminant flow-path databases from which the high-resolution dispersion nomographs are extracted. Other detailed models that can provide the same database could also be the source of data to build nomographs. If enough data were taken in field trials or experiments, equivalent to three-dimensional fields of key variables over the region, nomographs could then be made from field data^[3].

The four steps in generating and using dispersion nomographs are:

1. An accurate geometry database is compiled from light detection and ranging (LIDAR), stereo imagery, or shape files. The geometry database used by FAST3D-CT is a two-dimensional (typically one meter resolution) array that returns the heights of terrain, buildings, and trees, and surface composition in the computational domain.
2. Detailed 3D computational fluid dynamics calculations (FAST3D-CT) are repeated for 18 wind directions for the specified geometry and the results are captured in an extensive database. These simulations include the appropriate urban boundary layer for the region with realistic turbulent fluctuations imposed at the inflow boundaries. Multiple releases are tracked in each case as described above.
3. The salient features from the CFD database are distilled into Dispersion Nomograf data structures for rapid interactive access. Time integration is thus replaced by interpolations that capture the aerodynamic effects of the full urban geometry through the Nomograf tables.
4. The Nomograf tables are encrypted and input to CT-Analyst, an easy-to-use graphical user interface for instantaneous situational analysis. Plume computation, for example, takes less than 50 milliseconds.

B. The CT-Analyst[®] Emergency Assessment Tool

To solve the critical dilemma and to meet real operational requirements, NRL developed an integrated CBR emergency assessment tool that is much faster than current "common use" models while being more accurate. The focus is on situation assessment through sensor fusion of qualitative and incomplete data. A terrorist probably will not tell us the amount and location of an agent source or even what the agent is. Therefore we should not expect this information early enough for action in a crisis unless we somehow can generate what we need from the hints that will be available. The only existing

software tool with these capabilities is called CT-Analyst and is both zero-latency (meaning nearly zero computing delay) and high fidelity. CT-Analyst is entirely visual, i.e., "point-and-click," in application. Beta-test versions, implemented in modest laptop and workstation versions, treating all of the buildings and structures in a multiple-square-mile area of downtown, has been delivered to the cities of Chicago, New York, Houston, Washington DC, and to other officials in the Department of Defense. A corresponding capability has been delivered to civil emergency-management authorities in the District of Columbia. The Missile Defense Agency has incorporated CT-Analyst into its Post Engagement Ground Effects Model^[18] and a commercial implementation for law enforcement is marketed by Defense Group Incorporated^[19].

Each point in an urban area, if considered as a source location, has a downwind region called the footprint that can become contaminated by an airborne agent reaching that source point. Any selected location (considered as a site of interest) also has an upwind region (the danger zone) within which contaminant would have to be released to reach and contaminate that site. These two classes of regions are completely complementary, being effectively each other's inverse. All assessments in CT-Analyst are "computed" by manipulating these two distinct regions for sensor report locations, for selected site locations, and for source locations. The dispersion nomograf representation is designed to make these manipulations very fast while requiring only a minimum amount of tabulated data for each wind direction. The dispersion nomograf representation and processing algorithms also allow some new features. Multiple sensor fusion for instantaneous situation assessment is an automatic consequence of the nomograf representation. The methodology can accept qualitative and anecdotal input and does not require knowledge of a source location or even a source type or amount. A backtrack to unknown source locations is performed graphically with zero delay by overlap operations on the upwind danger zones of the "hot" and "cold" sensor reports.

Figure 2 shows a typical CT-Analyst display for an urban area, in this case a section of downtown Houston. The backtrack to the source based solely on sensor reports is shown in dark blue. Star-shaped nodes are sources, triangular and circular nodes are sensor reports, and square nodes indicate specific sites. When a source node is active it is colored light blue, as shown above. Footprints, plume envelopes, contaminant concentration plots, and escape routes can be displayed for sources by activating buttons on the lower portion of the CT-Analyst screen. Triangular sensor report nodes inside an active plume envelope are "hot" (red) while those still uncontaminated are "cold" (blue). Downwind consequence regions (for active "hot" reports) and

upwind backtrack estimates (for all active "hot" and "cold" reports) can be displayed for the active sensor nodes, indicated by filled triangles.

Contamination zones from down wind leakage and upwind danger zones can be plotted for all square site nodes (bright green when they are active). The diagonal purple lines are the recommended evacuation routes.

3. HPC Implementation of Data Generation for Nomographs

The Nunn-Lugar-Domenici Domestic Preparedness Program^[20] initially identified one hundred and twenty cities as likely terrorist targets. This number has since been increased to over 150. Military installations and other potential targets further increase this number. For each of these cities and installations, nomograf data has to be generated for each of eighteen wind angles and up to four environmental conditions. Each combination of wind angle and environmental condition requires a separate CFD run to obtain the required data for the corresponding nomograf. Clearly, this results in a large number of *independent* runs that will be required. In addition, the city can also be divided up into a number of distinct tiles. When treated separately, these tiles lead to even more independent CFD runs than can be executed in parallel.

In performing production runs to develop the necessary Dispersion Nomograf data sets, a number of levels of parallelism can be exploited to optimize the processing and permit the data sets to be developed in a rational sequence, working from the center of the city outward. Because of these multiple levels of parallelism, the version of the model (and the parallel architecture) used for each case only needs to be moderately scalable. Measures and metrics such as gigaflops, parallel-speed-up, etc., are largely academic. The key, and arguably the only metric of importance, is the overall time to solution. We must focus our efforts on reducing the time required to put in place a robust and accurate system for protecting our cities and military installations.

In order to generate all the data to cover 150 cities will require many independent large, but not huge, shared memory parallel jobs. In this application the scalability of individual jobs is not so critical, and an effective architecture would be a cluster of shared memory nodes, each with 16–32 processors. This problem is limited currently by processor speed and memory bandwidth, especially between processors on each node. In this case, other than for file management and subsequent nomograf generation, communication within the cluster is negligible. Such computers are readily available today.

Special cases will arise that need to be considered for detailed analysis. These studies may involve higher

resolution and include much more detailed and complex physics, especially if the agent is known and has complicated physics or chemistry. Agent fate and deposition may have to be considered. These cases will be far fewer in number but will be required due to special circumstances and will usually be time-critical. The individual runs for these cases must be completed as expeditiously as possible. Here, massive scalability becomes much more important. For the shared memory-based FAST3D-CT code, the ideal computer would have flat memory access from all processors. In the long range, it may be required to re-develop an up-to-date distributed memory version of FAST3D-CT.

A. The Current HPC Implementation of FAST3D-CT

Optimizing the sub-models in FAST3D-CT requires a number of different data structures for distributed memory parallel systems. Detailed simulations of buoyant and neutral gas contaminants, multi-group droplet problems, and multi-group particle sources for biological and radiological (“dirty bomb”) scenarios for example cause severe load-balancing problems for realistic problems in which much of the grid may have no contaminants at all. To provide a high degree of fidelity in solar deposition, a ray-trace algorithm was implemented so buildings and trees could cast realistic shadows. To keep this cost to a few percent of the overall running time, this piece of complex geometry physics was knowingly implemented in a manner only conducive to a shared-memory implementation.

The parallelization strategy adopted in FAST3D-CT is essentially loop-level parallelism controlled by OpenMP directives. However, these directives were placed such that the parallel regions were extended to encompass multiple loops. The outermost of the three-dimensional loops was parallelized if at all possible. The main computational kernel, LCPFCT^[15] was placed in parallel loops so that the overhead of parallelization is minimal. The limiting factor to parallel speed-up in the current implementation of FAST3D-CT is non-local memory access. While this can and is minimized by the first-touch strategy that we have adopted, the directionally split scheme used for fluid and contaminant transport effectively requires a partial transpose of the data at each timestep. Though a transpose is not used explicitly, data must be accessed with non-unity strides prior to performing the y- and z-direction integrations. The long strides required in the z-direction integrations results in cache line and translation lookup buffer misses, leading to poor performance. Performing a partial transpose explicitly for the z-direction integrations alleviates this. With this extra step, translation lookup buffer misses are completely eliminated.

The use of OpenMP does limit the parallel speedup possible in the FAST3D-CT code. OpenMP was selected because of the lower programming effort required due to the simpler program structure. This in turn eased debugging and allowed rapid insertion and testing of new physics models and algorithms. As was explained above, there is also a hierarchy of levels of parallelism in this problem that suggests optimal performance will result from exploiting only a modest level of parallelism for each run but executing the many required runs in parallel.

B. Future Direction

In the beginning of this section, we discussed the high performance computing requirements to develop nomograf representations for all the regions where CT-Analyst application could be necessary. This is the single largest cost and therefore the main deterrent to wider use of CT-Analyst. Reducing the computer requirements and thus the time delay to implement CT-Analyst is very important and thus the subject of continuing research and development. To this end we have been planning a turnkey nomograf generation system that can be run by relatively untrained personnel (not PhDs) on smaller HPC systems already present at a number of sites. The four stages in computing nomographs described above become four coupled processes in a single computer system. The most difficult of these four stages to automate is the first; an automatic software system that can prepare the geometry database required for the detailed LES simulations needed to prepare nomographs. Graphical tools will help but the system will still have to be keyed to one or two sources of geometry information such as LIDAR in standard formats.

Meanwhile, work continues on improving the speed of the FAST3D-CT computations themselves and a factor of two seems possible with no loss of computer accuracy for the second stage of the process. The LES runs can certainly be packaged and controlled by a graphical user interface to generate the eighteen input data streams, manage the data collected from the runs, and inform on progress. This same controller can also pipe the intermediate as well as final results into the nomograf generation software so that useable dispersion nomographs can be made accessible even before the longest 3D simulations are complete. Once a candidate nomograf data set has been produced, the turnkey system would automatically over-write earlier (lower-fidelity) approximations.

4. Conclusion

Physically realistic urban aerodynamics simulations are now possible but still require some compromises due

to time, computer, and manpower resource limitations. The necessary trade-offs result in sometimes using simpler models, algorithms, and geometry representations than we would wish. We have shown^[1,16] that the building and large-scale fluid dynamics effects that can be captured presently govern the turbulent dispersion, and thus expect that the computed predictions will get better in time because the MILES methodology is convergent when computational resolution can be improved. Inherent uncertainties in simulation inputs and model parameters beyond the environmental conditions also lead to errors that need to be further quantified by comparison with high quality reference data.

Using this HPC-based LES model as a detailed scenario generator, we have invented a process to make the 3D CFD really useful in real time for crisis managers in operational situations. As a bottom line, the increased speed and accuracy of using dispersion nomographs in CT-Analyst can reduce the number of people being exposed in urban CT scenarios, even for large crowds in the open, by 85 to 95% once an effective sensor or reporting network is in place. First responders and headquarters staff can use this tool for data fusion to give a minute-by-minute situation assessment. By performing all the major computing ahead of time on HPC computers well suited to the application, the results of a number of complete, high-resolution 3D simulations can be recalled for operational usage with no sensible delay for integration of even simple models. In this way we have solved the usual dilemma of more computer time being required to obtain better answers.

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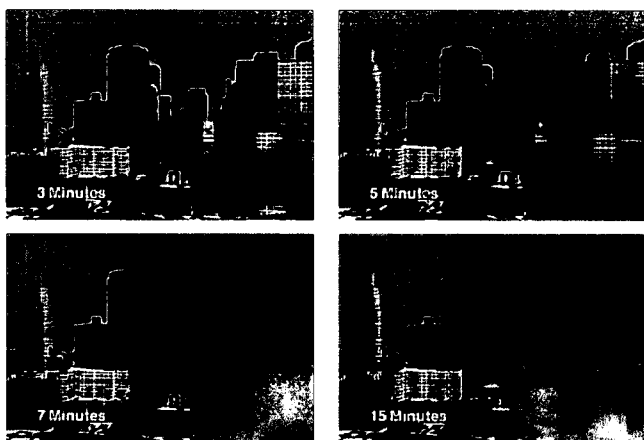


Figure 1. Contaminant dispersion from an instantaneous release in Times Square, New York City as predicted by the FAST3D-CT. The frames show concentrations at 3, 5, 7, and 15 minutes after release.

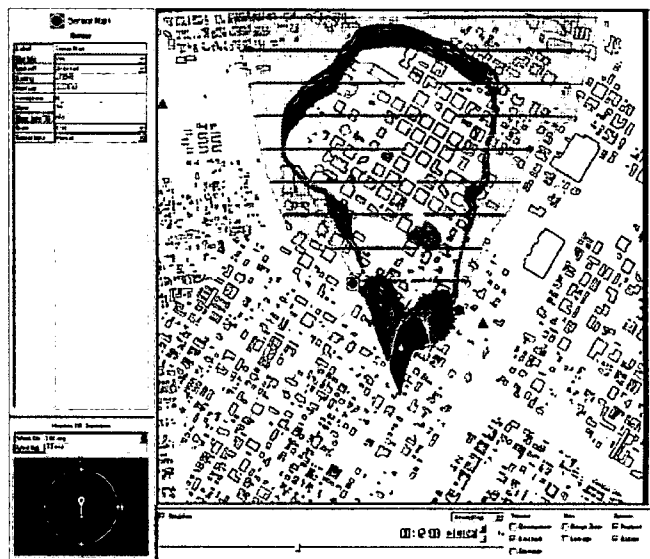


Figure 2. CT-Analyst display for downtown Houston showing contaminant concentration contours (yellow, green, and blue), contamination footprint (grey), and evacuation routes (magenta/purple lines). Backtrack region is shown in dark blue.